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Jacobian

Given a set $\mathbf{y} = \mathbf{f}(\mathbf{x})$ of n equations in n variables x_1, ..., x_n, written explicitly as

$$\mathbf{y} = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_n(\mathbf{x}) \end{bmatrix}, \tag{1}$$

or more explicitly as

$$\begin{cases} y_1 = f_1(x_1, \ldots, x_n) \\ \vdots \\ y_n = f_n(x_1, \ldots, x_n), \end{cases} \tag{2}$$

the Jacobian matrix, sometimes simply called "the Jacobian" (Simon and Blume 1994) is defined by

$$J(x_1, \ldots, x_n) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_n} \end{bmatrix}. \tag{3}$$

The determinant of J is the Jacobian determinant (confusingly, often called "the Jacobian" as well) and is denoted

$$J = \left| \frac{\partial(y_1, \ldots, y_n)}{\partial(x_1, \ldots, x_n)} \right|. \tag{4}$$

The Jacobian matrix and determinant can be computed using the *Mathematica* commands

```
JacobianMatrix[f_List?VectorQ, x_List] := Outer[D, f, x] /; Equal@@(Dimensions/@{f,x})
JacobianDeterminant[f_List?VectorQ, x_List] := Det[JacobianMatrix[f, x]] /;
  Equal @@ (Dimensions /@ {f, x})
```

Taking the differential

$$d\mathbf{y} = \mathbf{y}_{\mathbf{x}}\, d\mathbf{x} \tag{5}$$

shows that J is the determinant of the matrix $\mathbf{y}_{\mathbf{x}}$, and therefore gives the ratios of n-dimensional volumes (contents) in y and x,

$$dy_1 \ldots dy_n = \left| \frac{\partial(y_1, \ldots, y_n)}{\partial(x_1, \ldots, x_n)} \right| dx_1 \ldots dx_n \tag{6}$$

$|\partial(x_1,\ldots,x_n)|$

It therefore appears, for example, in the change of variables theorem.

The concept of the Jacobian can also be applied to n functions in more than n variables. For example, considering $f(u,v,w)$ and $g(u,v,w)$, the Jacobians

$$\frac{\partial(f,g)}{\partial(u,v)} \equiv \begin{vmatrix} f_u & f_v \\ g_u & g_v \end{vmatrix} \tag{7}$$

$$\frac{\partial(f,g)}{\partial(u,w)} \equiv \begin{vmatrix} f_u & f_w \\ g_u & g_w \end{vmatrix} \tag{8}$$

can be defined (Kaplan 1984, p. 99).

For the case of $n = 3$ variables, the Jacobian takes the special form

$$Jf(x_1,x_2,x_3) \equiv \left|\frac{\partial \mathbf{y}}{\partial x_1}\cdot\frac{\partial \mathbf{y}}{\partial x_2}\times\frac{\partial \mathbf{y}}{\partial x_3}\right|, \tag{9}$$

where $\mathbf{a}\cdot\mathbf{b}$ is the dot product and $\mathbf{b}\times\mathbf{c}$ is the cross product, which can be expanded to give

$$\left|\frac{\partial(y_1,y_2,y_3)}{\partial(x_1,x_2,x_3)}\right| \equiv \begin{vmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \frac{\partial y_1}{\partial x_3} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \frac{\partial y_2}{\partial x_3} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \frac{\partial y_3}{\partial x_3} \end{vmatrix}. \tag{10}$$

SEE ALSO: Change of Variables Theorem, Curvilinear Coordinates, Hessian, Implicit Function Theorem, Multivariable Calculus, Wronskian

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Gradshteyn, I. S. and Ryzhik, I. M. "Jacobian Determinant." §14.313 in *Tables of Integrals, Series, and Products, 6th ed.* San Diego, CA: Academic Press, pp. 1068-1069, 2000.

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Michael Conrad

May 1985 **Communications of the ACM**, Volume 28 Issue 5

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If the unique information-processing capabilities of protein enzymes could be adapted for computers, then evolvable, more efficient systems for such applications as pattern recognition and process control are in principle possible.

2 Stochastic roadmap simulation: an efficient representation and algorithm for analyzing molecular motion

Mehmet Serkan Apaydin, Douglas L. Brutlag, Carlos Guestrin, David Hsu, Jean-Claude Latombe

April 2002 **Proceedings of the sixth annual international conference on Computational biology**

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September 2004 **ACM Transactions on Mathematical Software (TOMS)**, Volume 30 Issue 3

Full text available: pdf(911.92 KB) Additional Information: full citation, abstract, references, index terms

ProtoMol is a high-performance framework in C++ for rapid prototyping of novel algorithms for molecular dynamics and related applications. Its flexibility is achieved primarily through the use of inheritance and design patterns (object-oriented programming). Performance is obtained by using templates that enable generation of efficient code for sections critical to performance (generic programming). The framework encapsulates important optimizations that can be used by developers, such as parall ...

Keywords: Fast electrostatic methods, incremental parallelism, molecular dynamics, multigrid, multiple time-stepping integration, object-oriented framework.

4 Algorithmic issues in modeling motion

Pankaj K. Agarwal, Leonidas J. Guibas, Herbert Edelsbrunner, Jeff Erickson, Michael Isard, Sariel Har-Peled, John Hershberger, Christian Jensen, Lydia Kavraki, Patrice Koehl, Ming Lin, Dinesh Manocha, Dimitris Metaxas, Brian Mirtich, David Mount, S. Muthukrishnan, Dinesh Pai, Elisha Sacks, Jack Snoeyink, Subhash Suri, Ouri Wolefson
December 2002 **ACM Computing Surveys (CSUR)**, Volume 34 Issue 4

Full text available: pdf(205.25 KB) Additional Information: full citation, abstract, references, citings, index terms

This article is a survey of research areas in which motion plays a pivotal role. The aim of the article is to review current approaches to modeling motion together with related data structures and algorithms, and to summarize the challenges that lie ahead in producing a more unified theory of motion representation that would be useful across several disciplines.

Keywords: Computational geometry, computer vision, mobile networks, modeling, molecular biology, motion modeling, physical simulation, robotoics, spatio-temporal databases

5 Demonstrating the scalability of a molecular dynamics application on a Petaflop computer

George S. Almasi, Călin Caşcaval, José G. Castaños, Monty Denneau, Wilm Donath, Maria Eleftheriou, Mark Giampapa, Howard Ho, Derek Lieber, José E. Moreira, Dennis Newns, Marc Snir, Henry S. Warren
June 2001 **Proceedings of the 15th international conference on Supercomputing**

Full text available: pdf(392.72 KB) Additional Information: full citation, abstract, references, citings, index terms

The IBM Blue Gene project has endeavored into the development of a cellular architecture computer with millions of concurrent threads of execution. One of the major challenges of this project is demonstrating that applications can successfully exploit this massive amount of parallelism. Starting from the sequential version of a well known molecular dynamics code, we developed a new application that exploits the multiple levels of parallelism in the Blue Gene cellular architecture. We perform ...

Keywords: Blue Gene, cellular architecture, massively parallel computing, molecular dynamics, performance evaluation

6 Visualization: Visualization of molecular quantum dynamics: a molecular visualization tool with integrated Web3D and haptics

R. Andrew Davies, Nigel W. John, John N. MacDonald, Keith H. Hughes

March 2005 **Proceedings of the tenth international conference on 3D Web technology**

Full text available: pdf(1.78 MB) Additional Information: full citation, abstract, references, index terms

The Department of Chemistry and the School of Informatics at the University of Wales, Bangor are working together to create tools for the visualization of molecular quantum dynamics. This paper presents the results of our initial work. A prototype Molecular Visualiser (MV) application has been developed based on Web3D standards, plus extensions for support of haptic interaction. MV provides the user with visualizations of molecular systems, potential energy surfaces, and wavepacket dynamics. The ...

Keywords: VRML, haptics, molecular quantum dynamics, visualization

7 Molecular simulation of rheological properties using massively parallel supercomputers

R. K. Bhupathiraju, S. T. Cui, S. Gupta, H. D. Cochran, P. T. Cummings

November 1996 **Proceedings of the 1996 ACM/IEEE conference on Supercomputing (CDROM) - Volume 00**

Full text available: pdf(120.44 KB) Additional Information: full citation, abstract, references, index terms

Advances in parallel supercomputing now make possible molecular-based engineering and science calculations that will soon revolutionize many technologies, such as those involving polymers and those involving aqueous electrolytes. We have developed a suite of message-passing codes for classical molecular simulation of such complex fluids and amorphous materials and have completed a number of demonstration calculations of problems of scientific and technological importance with each (describe ...

Keywords: Molecular dynamics, domain decomposition, molecular simulation, nonequilibrium, rheology

8 Simulating the dynamics of auroral phenomena

Gladimir V. G. Baranoski, Justin Wan, Jon G. Rokne, Ian Bell

January 2005 **ACM Transactions on Graphics (TOG)**, Volume 24 Issue 1

Full text available: pdf(214.56 KB) Additional Information: full citation, abstract, references, index terms

Simulating natural phenomena has always been a focal point for computer graphics research. Its importance goes beyond the production of appealing presentations, since research in this area can contribute to the scientific understanding of complex natural processes. The natural phenomena, known as the Aurora Borealis and Aurora Australis, are geomagnetic phenomena of impressive visual characteristics and remarkable scientific interest. Aurorae present a complex behavior that arises from intera ...

Keywords: Atmospheric effects, natural phenomena, plasma phenomena, rendering

9 A system for interactive molecular dynamics simulation

John E. Stone, Justin Gullingsrud, Klaus Schulten

March 2001 **Proceedings of the 2001 symposium on Interactive 3D graphics**

Full text available: pdf(129.46 KB) Additional Information: full citation, references, citings, index terms

Keywords: haptic feedback, molecular dynamics, steered molecular dynamics

10 Session P8: nature visualization: Visualizing dynamic molecular conformations

Johannes Schmidt-Ehrenberg, Daniel Baum, Hans Christian Hege

October 2002 **Proceedings of the conference on Visualization '02**

Full text available: pdf(2.72 MB) Additional Information: full citation, abstract, references, index terms

The bioactivity of a molecule strongly depends on its metastable conformational shapes and the transitions between these. Therefore, conformation analysis and visualization is a basic prerequisite for the understanding of biochemical processes.We present techniques for visual analysis of metastable molecular conformations. Core of these are flexibly applicable methods for alignment of molecular geometries, as well as methods for depicting shape and 'fuzziness' of metastable conformations. All an ...

Keywords: drug design, molecular conformation analysis, molecular modeling, uncertainty visualization

11 A modeling system based on dynamic constraints

Ronen Barzel, Alan H. Barr

June 1988 **ACM SIGGRAPH Computer Graphics , Proceedings of the 15th annual conference on Computer graphics and interactive techniques**, Volume 22 Issue 4

Full text available: pdf(4.29 MB) Additional Information: full citation, abstract, references, citings, index terms

We present "dynamic constraints," a physically-based technique for constraint-based control of computer graphics models. Using dynamic constraints, we build objects by specifying geometric constraints; the models assemble themselves as the elements move to satisfy the constraints. The individual elements are rigid bodies which act in accordance with the rules of physics, and can thus exhibit physically realistic behavior. To implement the constraints, a set of "constraint forces" is found, which ...

Keywords: contraints, dynamics, modeling, simulation

12 Animation of dynamic legged locomotion

Marc H. Raibert, Jessica K. Hodgins

July 1991 **ACM SIGGRAPH Computer Graphics , Proceedings of the 18th annual conference on Computer graphics and interactive techniques**, Volume 25 Issue 4

Full text available: pdf(1.72 MB) Additional Information: full citation, abstract, references, citings, index terms

This paper is about the use of control algorithms to animate dynamic legged locomotion. Control could free the animator from specifying the details of joint and limb motion while producing both physically realistic and natural looking results. We implemented computer animations of a biped robot, a quadruped robot, and a kangaroo. Each creature was modeled as a linked set of rigid bodies with compliant

actuators at its joints. Control algorithms regulated the running speed, organized use of the l ...

Keywords: computer animation, dynamical simulation, legged locomotion, motion control, physically realistic modeling, robotics

13 VRML molecular dynamics trajectories 

Geoff Leach, James Gilbert

February 1999 **Proceedings of the fourth symposium on Virtual reality modeling language**

Full text available: pdf(2.25 MB) Additional Information: full citation, references, index terms

Keywords: VRML, compression, molecular dynamics, scientific visualisation

14 Scalable molecular dynamics for large biomolecular systems 

Robert K. Brunner, James C. Phillips, Laxmikant V. Kale

November 2000 **Proceedings of the 2000 ACM/IEEE conference on Supercomputing (CDROM)**

Full text available: pdf(211.89 KB) Additional Information: full citation, abstract, references, citings, index terms

Publisher Site

We present an optimized parallelization scheme for molecular dynamics simulations of large biomolecular systems, implemented in the production-quality molecular dynamics program NAMD. With an object-based hybrid force and spatial decomposition scheme, and an aggressive measurement-based predictive load-balancing framework, we have attained speeds and speedups that are much higher than any reported in literature so far. The paper first summarizes the broad methodology we are pu ...

15 Computational fluid dynamics in a traditional animation environment 

Patrick Witting

July 1999 **Proceedings of the 26th annual conference on Computer graphics and interactive techniques**

Full text available: pdf(734.22 KB) Additional Information: full citation, references, citings, index terms

Keywords: animation, animation systems, applications, fluid simulations, natural phenomena, numerical analysis, physically based animation, physically based modeling, scientific visualization, texture mapping

16 Modeling the motion of a hot, turbulent gas 

Nick Foster, Dimitris Metaxas

August 1997 **Proceedings of the 24th annual conference on Computer graphics and interactive techniques**

Full text available: pdf(5.92 MB) Additional Information: full citation, references, citings

Keywords: animation, convection, gas simulations, gaseous phenomena, physics-based modeling, smoke, steam, turbulent flow

17 Simulation, motion capture, editing: Modeling tension and relaxation for computer animation

Michael Neff, Eugene Fiume

July 2002 **Proceedings of the 2002 ACM SIGGRAPH/Eurographics symposium on Computer animation**

Full text available: pdf(3.44 MB) Additional Information: full citation, abstract, references, citings, index terms

The use of tension and relaxation in the muscles of real creatures gives rise to nuanced motion that conveys emotion or intent. Artists have long exploited knowledge of this in traditional animation and other areas, but it has been both overlooked and difficult to achieve in physically based animation. The robotically stiff motion that has come to typify physically based approaches belies the fact that dynamics has much to offer in facilitating far more subtle motion in which animators could fre ...

Keywords: animation, human body simulation, physically based animation

18 Parallel approaches to short range molecular dynamics simulations

Pablo Tamayo, Jill P. Mesirov, Bruce M. Boghosian

August 1991 **Proceedings of the 1991 ACM/IEEE conference on Supercomputing**

Full text available: pdf(818.30 KB) Additional Information: full citation, references, citings, index terms

19 Simulation and preferences: Virtual spring manipulators for particle steering in molecular dynamics on the responsive workbench

Michal Koutek, Jeroen van Hees, Frits H. Post, A. F. Bakker

May 2002 **Proceedings of the workshop on Virtual environments 2002**

Full text available: pdf(6.52 MB) Additional Information: full citation, abstract, references, citings

In this paper we present new virtual spring manipulator-based tools for steering particles in molecular dynamics simulations in virtual environments. We briefly overview the MolDRIVE system, our visualization and computational steering environment for molecular dynamics real-time simulations, which is the platform for our particle steering implementation.Our study concentrates on visual feedback tools. We compare a basic virtual particle steering method with two other methods using a spring mani ...

20 An 8.61 Tflop/s molecular dynamics simulation for NaCl with a special-purpose computer: MDM

Tetsu Narumi, Atsushi Kawai, Takahiro Koishi

November 2001 **Proceedings of the 2001 ACM/IEEE conference on Supercomputing (CDROM)**

Full text available: pdf(1.19 MB) Additional Information: full citation, abstract, references, index terms

We performed molecular dynamics (MD) simulation of 33 million pairs of NaCl ions with the Ewald summation and obtained a calculation speed of 8.61 Tflop/s. In this calculation we used a special-purpose computer, MDM, which we have developed for the calculations of the Coulomb and van der Waals forces. The MDM enabled us to perform large scale MD simulations without truncating the Coulomb force. It is composed of MDGRAPE-2, WINE-2 and a host computer. MDGRAPE-2 accelerates the calculation for rea ...

Keywords: ewald method, molecular dynamics simulation, special-purpose computer

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81 An analytic approach to significance assessment in local sequence alignment with gaps

R. Bundschuh

April 2000 **Proceedings of the fourth annual international conference on Computational molecular biology**

Full text available: pdf(974.15 KB) Additional Information: full citation, abstract, references, citings

A detailed study of the Smith-Waterman alignment algorithm is performed in order to find an analytical approach to the problem of assessing the statistical significance of local alignments with gaps. The significance is shown to be given in terms of an eigenvalue equation which captures the dynamics of the much simpler global alignment algorithm. This eigenvalue equation is then explicitly solved for a simple scoring system and the resulting significance estimations are verified by a comparis ...

Keywords: Gumbel distribution, sequence alignment, statistical significance

82 Protein structure determination using protein threading and sparse NMR data (extended abstract)

Ying Xu, Dong Xu, Oakley H. Crawford, J. Ralph Einstein, Engin Serpersu

April 2000 **Proceedings of the fourth annual international conference on Computational molecular biology**

Full text available: pdf(663.42 KB) Additional Information: full citation, abstract, references, citings

It is well known that the NMR method for protein structure determination applies to small proteins and that its effectiveness decreases very rapidly as the molecular weight increases beyond about 30 kD. We have recently developed a method for protein structure determination that can fully utilize partial NMR data as calculation constraints. The core of the method is a threading algorithm that guarantees to find a globally optimal alignment between a query sequence and a template structure, ...

***Keywords**: NMR, energy minimization, fold recognition, protein structure*

determination, protein threading

83 HPFBench: a high performance Fortran benchmark suite

Y. Charlie Hu, Guohua Jin, S. Lennart Johnsson, Dimitris Kehagias, Nadia Shalaby

March 2000 **ACM Transactions on Mathematical Software (TOMS)**, Volume 26 Issue 1

Full text available: pdf(274.52 KB) Additional Information: full citation, abstract, references, citings, index terms

The high performance Fortran (HPF) benchmark suite HPFBench is designed for evaluating the HPF language and compilers on scalable architectures. The functionality of the benchmarks covers scientific software library functions and application kernels that reflect the computational structure and communication patterns in fluid dynamic simulations, fundamental physics, and molecular studies in chemistry and biology. The benchmarks are characterized in terms of FLOP count, memory usage, communi ...

Keywords: benchmarks, compilers, high performance Fortran

84 Pattern matching in dynamic texts

Stephen Alstrup, Gerth Stølting Brodal, Theis Rauhe

February 2000 **Proceedings of the eleventh annual ACM-SIAM symposium on Discrete algorithms**

Full text available: pdf(985.73 KB) Additional Information: full citation, references, citings, index terms

85 Algorithmic strategies in combinatorial chemistry

Deborah Goldman, Sorin Istrail, Giuseppe Lancia, Antonio Piccolboni, Brian Walenz

February 2000 **Proceedings of the eleventh annual ACM-SIAM symposium on Discrete algorithms**

Full text available: pdf(940.84 KB) Additional Information: full citation, references, index terms

86 Computational fluid dynamics in a traditional animation environment

Patrick Witting

July 1999 **Proceedings of the 26th annual conference on Computer graphics and interactive techniques**

Full text available: pdf(734.22 KB) Additional Information: full citation, references, citings, index terms

Keywords: animation, animation systems, applications, fluid simulations, natural phenomena, numerical analysis, physically based animation, physically based modeling, scientific visualization, texture mapping

87 Distance browsing in spatial databases

Gísli R. Hjaltason, Hanan Samet

June 1999 **ACM Transactions on Database Systems (TODS)**, Volume 24 Issue 2

Full text available: pdf(460.81 KB) Additional Information: full citation, abstract, references, citings, index terms

We compare two different techniques for browsing through a collection of spatial objects stored in an R-tree spatial data structure on the basis of their distances from an arbitrary spatial query object. The conventional approach is one that makes use of a k-nearest neighbor algorithm where k is known prior to the invocation of the algorithm. Thus if m < k neighbors are needed, the k-nearest neighbor alg ...

Keywords: R-trees, distance browsing, hiearchical spatial data structures, nearest neighbors, ranking

88 Complexity theory column 24: Biomolecular computing: recent theoretical and experimental advances

Lane A. Hemaspaandra

June 1999 **ACM SIGACT News**, Volume 30 Issue 2

Full text available: pdf(573.28 KB) Additional Information: full citation, abstract, references

And so summer comes around again. What a good time to relax on the beach (with your theorem notebook), to go on that long-planned family vacation (certainly with your theorem notebook, and don't forget to bring the family) and, above all, to catch up on all the papers and progress that have been piling up during the academic year on your "if only I had the time" list.The current column may save you some time on this! In 1997, Mitsunori Ogihara and Animesh Ray, jointly with Kimberly Smith, wrote ...

89 Improving cache performance in dynamic applications through data and computation reorganization at run time

Chen Ding, Ken Kennedy

May 1999 **ACM SIGPLAN Notices , Proceedings of the ACM SIGPLAN 1999 conference on Programming language design and implementation**, Volume 34 Issue 5

Full text available: pdf(1.54 MB) Additional Information: full citation, abstract, references, citings, index terms

With the rapid improvement of processor speed, performance of the memory hierarchy has become the principal bottleneck for most applications. A number of compiler transformations have been developed to improve data reuse in cache and registers, thus reducing the total number of direct memory accesses in a program. Until now, however, most data reuse transformations have been *static*---applied only at compile time. As a result, these transformations cannot be used to optimize irregular and ...

90 Searching gene transfers on Bacillus subtilis using hidden Markov models

Laurent Bize, Florence Muri, Franck Samson, François Rodolphe, S. Dusko Ehrlich, Bernard Prum, Philippe Bessières

April 1999 **Proceedings of the third annual international conference on Computational molecular biology**

Full text available: pdf(738.72 KB) Additional Information: full citation, references, index terms

91 Large scale molecular dynamics simulations with fast multipole implementations

Zhiqiang Wang, James A. Lupo, Alan M. McKenney, Ruth Pachter
January 1999 **Proceedings of the 1999 ACM/IEEE conference on Supercomputing (CDROM)**
Full text available: pdf(748.81 KB) Additional Information: full citation, references, citings, index terms

92 A unifying data structure for hierarchical methods
Faith E. Sevilgen, Srinivas Aluru
January 1999 **Proceedings of the 1999 ACM/IEEE conference on Supercomputing (CDROM)**
Full text available: pdf(88.91 KB) Additional Information: full citation, references, index terms

93 Parallel implementation of a molecular dynamics simulation program
Alan Mink, Christophe Bailly
December 1998 **Proceedings of the 30th conference on Winter simulation**
Full text available: pdf(100.62 KB) Additional Information: full citation, references, index terms

94 Recipes for adjoint code construction
Ralf Giering, Thomas Kaminski
December 1998 **ACM Transactions on Mathematical Software (TOMS)**, Volume 24 Issue 4
Full text available: pdf(301.79 KB) Additional Information: full citation, abstract, references, citings, index terms

Adjoint models are increasingly being developed for use in meteorology and oceanography. Typical applications are data assimilation, model tuning, sensitivity analysis, and determination of singular vectors. The adjoint model computes the gradient of a cost function with respect to control variables. Generation of adjoint code may be seen as the special case of differentiation of algorithms in reverse mode, where the dependent function is a scalar. The described method for adjoint code gene ...

Keywords: adjoint model, adjoint operator, automatic differentiation, computational differentiation, data assimilation, differentiation of algorithms, implicit functions, inverse modeling, optimization, reverse mode

95 A parallel rendezvous algorithm for interpolation between multiple grids
Steve Plimpton, Bruce Hendrickson, James Stewart
November 1998 **Proceedings of the 1998 ACM/IEEE conference on Supercomputing (CDROM)**
Full text available: html(37.23 KB) Additional Information: full citation, abstract, references, citings

A number of computational procedures employ multiple grids on which solutions are computed. For example, in multi-physics simulations a primary grid may be used to compute mechanical deformation of an object while a secondary grid is used for thermal conduction calculations. When modeling coupled thermo-mechanical effects, solution data must be interpolated back and forth between the grids each timestep. On a parallel machine, this grid transfer operation can be challenging if the two grids are ...

Keywords: grid transfer, load-balancing, multi-physics, multigrid, parallel computing

96 A hierarchical load-balancing framework for dynamic multithreaded computations

Vijay Karamcheti, Andrew A. Chien

November 1998 **Proceedings of the 1998 ACM/IEEE conference on Supercomputing (CDROM)**

Full text available: pdf(120.01 KB) Additional Information: full citation, abstract, references

High-level parallel programming models that support dynamic fine-grained threads in a global object space, are becoming increasingly popular for expressing irregular applications based on sophisticated adaptive algorithms and pointer-based data structures. However, implementing these multithreaded computations on scalable parallel machines poses significant challenges, particularly with respect to load-balancing. Load-balancing techniques must simultaneously incur low overhead to support fine-gr ...

97 Application level scheduling of gene sequence comparison on metacomputers

Neil Spring, Rich Wolski

July 1998 **Proceedings of the 12th international conference on Supercomputing**

Full text available: pdf(1.35 MB) Additional Information: full citation, references, citings, index terms

98 On approximating arbitrary metrices by tree metrics

Yair Bartal

May 1998 **Proceedings of the thirtieth annual ACM symposium on Theory of computing**

Full text available: pdf(4.11 MB) Additional Information: full citation, references, citings, index terms

99 Using prediction to accelerate coherence protocols

Shubhendu S. Mukherjee, Mark D. Hill

April 1998 **ACM SIGARCH Computer Architecture News , Proceedings of the 25th annual international symposium on Computer architecture,** Volume 26 Issue 3

Full text available: pdf(1.71 MB) Additional Information: full citation, abstract, references, citings, index terms

Publisher Site

Most large shared-memory multiprocessors use directory protocols to keep per-processor caches coherent. Some memory references in such systems, however, suffer long latencies for misses to remotely-cached blocks. To ameliorate this latency, researchers have augmented standard coherence protocols with optimizations for specific sharing patterns, such as read-modify-write, producer-consumer, and migratory sharing. This paper seeks to replace these directed solutions with general prediction logic t ...

100 An algorithm for finding novel gapped motifs in DNA sequences

Emily Rocke, Martin Tompa

March 1998 **Proceedings of the second annual international conference on Computational molecular biology**

Full text available: pdf(643.93 KB) Additional Information: full citation, references, citings, index terms

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